Electron dynamics and dynamic localization in asymmetric periodic potentials

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We consider the dynamics of electrons in asymmetric periodic potentials in ac electric fields. It is shown that the conditions for dynamic localization are not affected by the asymmetry of the potential and that the same ac field yields dynamic localization for any potential. However, the asymmetry does affect the general dynamics and must be included explicitly in dynamical calculations. We also show that the condition for dynamic localization in any potential can be interpreted as the requirement that the electron spend equal time at every point in the first Brillouin zone.

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Dynamic localization (DL) occurs when electrons in a periodic potential are localized in the presence of a periodic ac electric field. DL manifests itself through the return of the electron to its initial state after integer numbers of periods of the applied field. For a sinusoidal electric field (period τ, amplitude E_0) it has been shown that for certain ratios of E_0 and τ, the electrons are dynamically localized.[1–3] In deriving this result, the authors make the following approximations: they (1) employ the nearest-neighbor tight-binding (NNTB) approximation, (2) include only a single band in the calculation, and (3) ignore decoherence and dephasing processes that lead to homogeneous and inhomogeneous broadening. In addition, these authors, as well as most authors calculating ultrafast intraband dynamics in semiconductor superlattices,[4] (4) disregard the effects of any asymmetry in the periodic potential on electron dynamics.

More recently it was shown[5–7] that under the same approximations, many other periodic electric fields also lead to DL. In particular, Domachuk *et al.*[6] showed that almost all fields that are symmetric under time inversion, including the sinusoidal field, lead to DL in the NNTB approximation for some field amplitudes. However, DL does not occur beyond the NNTB approximation for almost any of these fields.[8–10] In contrast, Zhu *et al.*[7] showed that a periodic *square-wave* field can lead to exact dynamic localization (EDL): dynamic localization for arbitrary band structures and thus not just in the NNTB limit, thereby relaxing approximation (1).

A systematic study of EDL,[10] under the conditions (2)–(4) above, showed that EDL can only occur in electric fields that are discontinuous, such as the square wave mentioned above.[7] More generally, fields that lead to EDL must satisfy[10]

$$\beta_p(\tau)=0 \tag{1}$$

for all positive integer p, where τ is period of the ac electric field $E(t)$, and

$$\beta_p(t)\equiv\int_0^t e^{-ip\gamma(t')}dt', \tag{2}$$

where

$$\gamma(t)\equiv\frac{ed}{\hbar}\int_0^t E(t')dt'. \tag{3}$$

Here, e is the magnitude of the electron charge, d is the spatial period of the potential, and $\hbar$ is Planck's constant. The dimensionless quantity $\gamma(t)$ can be interpreted as the area of the electric field. As shown below, it also corresponds to a displacement in reciprocal space. In the NNTB approximation, DL requires only that $\beta_1(\tau)=0$. Previously,[10] we showed that requiring that Eq. (1) be satisfied for *all* $p\neq 0$ is equivalent to the condition

$$\tau=2\pi\sum_{m,j}|\dot{\gamma}(t_{jm})|^{-1}, \tag{4}$$

where the dot indicates a time derivative and the summation is over all times within a period τ at which $\gamma(t_{jm})=x+2\pi m$ $(-\pi\leqslant x<\pi)$. Here the j's count the roots of this equation for fixed m, as illustrated in Fig. 1 for one value of x. EDL thus requires that the sum of the absolute values of

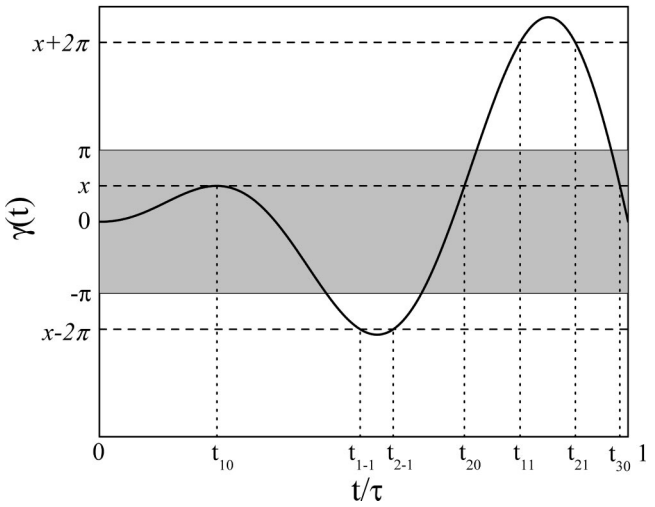

FIG. 1. Electric-field area γ vs time for a general ac electric field. Indicated are the t_{jm}, that enter Eq. (4), for one value of $\gamma=x$ (modulo 2π) (see dashed lines). The gray region indicates the first Brillouin zone.

the inverses of $\dot{\gamma}(t_{jm})$ at times where $\gamma(t_{jm})=x$ (modulo 2π) takes the value $\tau/(2\pi)$, independent of x (see Fig. 1). This leads to the requirement that the ac field must be discontinuous at all changes in its sign and must have an area between adjacent discontinuities that is an integer multiple of $2\pi\hbar/ed$.[6,10]

Here we generalize our previous results on EDL to potentials without inversion symmetry, thus dealing with condition (4). We find that the condition for EDL is identical for symmetric and asymmetric potentials, but that one must be careful when calculating the dynamics. Given the robustness of the results, it seems that there must be a simple physical interpretation of the requirement for EDL. The interpretation for the square-wave field was given previously.[10,11] Here we show that for general ac fields, if EDL is to occur, the electron must spend the same amount of time at all points in the first Brillouin zone.

We now examine the electron dynamics in a general asymmetric potential. We consider an electron in a one-dimensional periodic potential without inversion symmetry. We adopt a one-band model, ignore dephasing/decoherence effects [approximations (2) and (3)], and denote the Hamiltonian by H_0. We take the dispersion relation and Wannier functions for the lowest band of H_0 to be $\epsilon(k)$ and $|a_n\rangle$, respectively, where k is the electron's crystal momentum and n indicates the site where the Wannier function is centered. The Wannier functions $|a_n\rangle$ are expanded in terms of the Bloch states $|\psi_k\rangle$ of the band as

$$|a_n\rangle=\frac{1}{\sqrt{N}}\sum_k e^{-iknd}|\psi_k\rangle. \tag{5}$$

In the presence of the ac electric field $E(t)$ the full Hamiltonian is $H=H_0+eE(t)z$. We now expand the state ket $|\Psi(t)\rangle$ for the electron in the basis of the Wannier functions,

$$|\Psi(t)\rangle=\sum_n B_n(t)|a_n\rangle. \tag{6}$$

Using this into the Schrödinger equation, we obtain evolution equations for the expansion coefficients $B_n(t)$,

$$i\hbar\dot{B}_n=\sum_m B_m[\varepsilon_{n-m}+eE(t)W_{m-n}]+nedE(t)B_n. \tag{7}$$

Here, the ε_n are the Fourier coefficients of the band ($\varepsilon_n \equiv\Sigma_k\epsilon(k)\exp[ikd]$) and W_p is the matrix element of z,

$$W_p\equiv\langle a_0|z|a_p\rangle. \tag{8}$$

It can be shown by direct substitution that the solution to Eq. (7) is

$$B_n(t)=\exp\{-i[\varepsilon_0 t/\hbar+(n+W_0/d)\gamma(t)]\}$$
$$\times\sum_m A_{n-m}(t)B_m(0), \tag{9}$$

where

$$A_m(t)=\int_{-\pi}^{\pi}\frac{dx}{2\pi}\exp\left\{imx-i\sum_{p\neq 0}\frac{\varepsilon_{-p}}{\hbar}\tilde{\beta}_p(t)e^{ipx}\right\}, \tag{10}$$

and

$$\tilde{\beta}_p(t)\equiv\beta_p(t)+i\frac{\hbar W_p}{pd\varepsilon_{-p}}[\dot{\beta}_p(t)-1]. \tag{11}$$

To our knowledge, this is the first time this general solution has been presented.

Because the phases of the $|\psi_k\rangle$ can be chosen arbitrarily, the Wannier functions are not unique, and Wannier functions with widely differing properties may be constructed for a given band. The Wannier functions and the dipole matrix elements between different Wannier functions have been examined by many authors.[12–15] For one-dimensional symmetric potentials, Kohn[12] showed that Wannier functions with $W_p=0$ can be constructed by choosing the Bloch function phase such that $\langle z=0|\psi_k\rangle$ is real, where the origin of z is chosen such that $W_0=0$. We refer to the Wannier functions that result from this procedure as the Kohn-recipe basis (KRB). In all previous works where symmetric potentials were implicitly or explicitly considered, the authors have simply set $W_p=0$. If $W_p=0$, then $\beta(t)=\tilde{\beta}(t)$, and we obtain the solution reported previously for symmetric potentials.[7,10] More recently, it was shown that for a general, asymmetric, one-dimensional system, one can construct Wannier functions for which $W_p=0$, and that these functions are real and maximally localized.[15] Here we review these results, present a simple procedure for calculating this basis, and examine the effects of neglecting the W_p in a basis that is not the maximally localized basis (MLB).

Using Eq. (5), the matrix elements W_p are given by

$$W_p=\frac{1}{N}\sum_{k,k'}e^{-ik'pd}\langle\psi_k|z|\psi_{k'}\rangle. \tag{12}$$

Following Blount,[13] the Bloch-function matrix element of z can be expressed as

$$\langle\psi_k|z|\psi_{k'}\rangle=i\frac{2\pi}{L}\frac{\partial}{\partial k}\delta(k-k')+\frac{2\pi}{L}Z(k)\delta(k-k'), \tag{13}$$

where

$$Z(k)\equiv i\int u_k^*(z)\frac{\partial}{\partial k}u_k(z)dz, \tag{14}$$

where $u_k(z)$ is the periodic part of the Bloch function. We now define a set of Bloch states, $|\tilde{\psi}_k\rangle$, that differ from the original ones only by k-dependent phase factors: $|\tilde{\psi}_k\rangle \equiv e^{i\phi(k)}|\psi_k\rangle$. Using this and Eqs. (12) and (13), we obtain for the matrix element $\tilde{W}_p$ of z in the new Wannier function basis

$$\tilde{W}_p=W_p-\frac{d}{2\pi}\int_{-\pi/d}^{\pi/d}dke^{-ikpd}\phi'(k). \tag{15}$$

If we now choose

$$\phi(k)=2\sum_{m=1}^{\infty}\frac{W_m}{md}\sin(kmd), \tag{16}$$

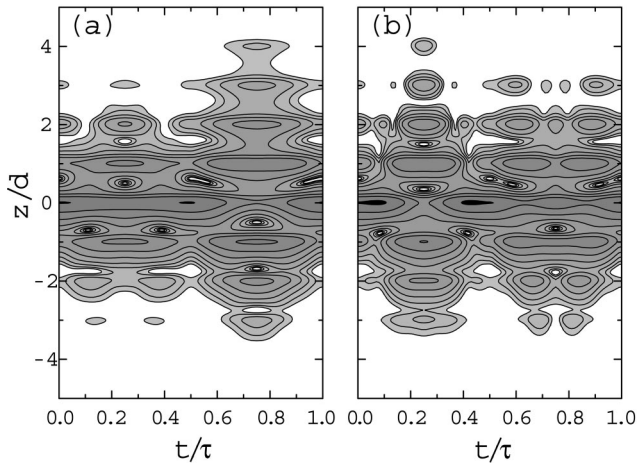

FIG. 2. Probability density (log scale) vs time for the asymmetric GaAs/$Ga_xAl_{1-x}As$ superlattice described in the text. The correct evolution is shown in (a), while the evolution using the KRB with the W_p incorrectly set to zero is shown in (b).

then $\tilde{W}_p=0$ for $p>0$. But, we can always choose our original Bloch functions such that $\psi_{-k}(z)=\psi_k^*(z)$. From Eq. (5) it then follows that the $a_p(z)$ are real and that hence the W_p are real. Using this in Eq. (8), we see that $W_{-p}=W_p$. Thus using $\phi(k)$ defined in Eq. (16), we have $\tilde{W}_p=0$ for $p\neq 0$. Finally, by choosing the appropriate origin for z, we can also choose $\tilde{W}_0=0$.

Since the form of the evolution equation (7) is identical for symmetric and asymmetric potentials if one uses the MLB (where $\tilde{W}_p=0$), EDL occurs in any potential (symmetric or asymmetric) for *exactly the same ac electric fields*. Moreover, the procedure for finding electric fields that lead to dynamic localization[10] applies equally to symmetric *and asymmetric* potentials: the fields must satisfy Eq. (4). Thus even if the W_p in the dynamical equation were to be ignored mistakenly, the equations would still yield EDL. However, the dynamics of the electrons between the times at which they are localized would not be correct. We now address this issue.

The MLB is not an obvious one, and one may simply want to use the KRB to calculate the dynamics. The dynamics of the electrons calculated using the MLB and KRB with corresponding W_p must be exactly the same if the same initial state $|\Psi(0)\rangle$ is used. However, one must not neglect the W_p in the calculation using the KRB for an asymmetric potential. To demonstrate this, we consider an asymmetric GaAs/$Ga_xAl_{1-x}As$ superlattice structure with a barrier thickness of 2.0 nm, and a well that has a 7.5 nm region at a potential 200 meV below the barrier and a 2.5 nm region at a potential 350 meV below the barrier. The effective electron mass is 0.067 that of the free electron mass. We take the ac field to be the minimum-amplitude square-wave ac field that yields EDL,[10] for which $E_0=2\hbar\omega/ed$, where $\omega=2\pi/\tau$, and $\tau=825$ fs. We employ the KRB Wannier functions. In a symmetric potential this would yield $W_p=0$ for all p, but for this asymmetric structure, the W_p are nonzero for $p\neq 0$. In Fig. 2(a) we present the evolution of the probability density with the W_p included for the initial condition that the electron is in the $n=0$ Wannier function of the MLB. In Fig. 2(b), we present the evolution as calculated again in the KRB, but with the W_p incorrectly set to zero. This is the result one would obtain if one ignored the asymmetry of the potential and simply used the KRB. Note that the evolution is strongly affected by the W_p. This demonstrates the importance of the inclusion of the W_p in any dynamical calculations. Similarly, if the calculation is done in the Bloch basis, one must correspondingly either choose the phases of the Bloch states according to Eq. (16) or else explicitly include the $Z(k)$ in the equations of motion.

Having shown that Eq. (4) is the requirement for dynamic localization for *any* periodic potential, we now turn to its physical interpretation. In the presence of an electric field, the well-known semiclassical evolution equation for the average crystal momentum of the wave packet, k, is $\hbar\dot{k}=eE(t)$. Using Eq. (3), we then obtain

$$k(t)=k_0+\gamma(t)/d, \tag{17}$$

where k_0 is the value of k at $t=0$. Thus, apart from a factor $1/d$, $\gamma(t)$ gives the electron displacement in reciprocal space. An electron exactly traverses the Brillouin zone once, when γ increases by 2π. Thus the different m that arise in the application of Eq. (4) correspond to positions in reciprocal space that differ by a reciprocal lattice vector. Since $\gamma(t)$ gives the displacement of electrons in reciprocal space, $\dot{\gamma}(t)$, again apart from a factor $1/d$, gives their "velocity" dk/dt in reciprocal space. Thus $\Delta k d/\dot{\gamma}$ corresponds to the time required to cross a reciprocal space interval of length Δk.

The interpretation of Eq. (4) can now be understood by referring to Fig. 1. The times t_{jm} correspond to the times at which γ (and hence k) takes a particular value x (modulo 2π). Hence, they correspond to the times that a particular position in the Brillouin zone is visited during a period of the ac field. These visits can be of two types: they may be due to the electron returning to the same k within the first Brillouin zone (corresponding to different j in t_{mj}), or they may be due to arrival of the electron at the position $k+2m\pi$ in the $m+1$ Brillouin zone (corresponding to different m in t_{mj}). At each visit, the time that the electron spends within an interval Δk about $k=\gamma(t_{jm})$ is $\Delta k d/|\dot{\gamma}(t_{jm})|$. Note that the absolute value is taken since the direction in which the electron travels does not matter. As $\Delta k\to 0$, Eq. (4) corresponds to the requirement that, during one period of the applied ac electric field, the electron spends an equal amount of time at each position in the first Brillouin zone.

One can draw two conclusions from the requirement that electrons spend equal time everywhere in the Brillouin zone. The first is that the initial condition does not matter. The second is that, since the electron spends equal time at each position, the contribution to the electron dynamics associated with a position k in the Brillouin zone is exactly canceled by that contribution at $-k$. Therefore, irrespective of the initial condition, after an integer number of field periods each electron ends up at its initial position, and *the electron* is thus dynamically localized. This last point can be made more clear by a semiclassical analysis. Consider the small dis-

placement Δz that the electron undergoes while within a small range Δk about k. The second semiclassical equation of motion gives $dz/dt=(1/\hbar)\partial\epsilon/\partial k$ for the average position of the electron. Using this relation and summing over all instances that the electron is within Δk of k, we obtain for the displacement Δz

$$\Delta z=\frac{1}{\hbar}\sum_{t_{jm}}\frac{\partial\epsilon[k(t_{jm})]}{\partial k}\Delta t=\frac{1}{\hbar}\frac{\partial\epsilon(k)}{\partial k}\Delta k\sum_{t_{jm}}\frac{d}{|\dot{\gamma}(t_{jm})|}. \tag{18}$$

Therefore, if the electric field satisfies the condition for dynamic localization [Eq. (4)], we find

$$\Delta z=\frac{d}{\hbar\omega}\frac{\partial\epsilon(k)}{\partial k}\Delta k, \tag{19}$$

where $\omega\equiv 2\pi/\tau$. Taking Δk to be an infinitesimal and integrating this from 0 to k, we obtain

$$z(k)=z_0+d\frac{\epsilon(k)}{\hbar\omega}. \tag{20}$$

Since $k(\tau)=k(0)$, the electron returns to its initial position at $t=\tau,2\tau,\ldots$ irrespective of the band structure or the initial conditions. More generally, the electron actually returns to its initial *state* at these times and is therefore dynamically localized.

Based on this interpretation of Eq. (4) we find that dynamic localization in a square-wave electric field corresponds to each position in the Brillouin zone being visited an equal number of times, and that each time the electron is traveling at the same speed in reciprocal space. For more general fields leading to EDL, the velocity in reciprocal space may vary, or the number of times that different positions are visited may vary, but the *total* time spent everywhere is nonetheless the same. The area condition that was noted earlier[10] corresponds to requiring that *all positions* in the Brillouin zone are visited, not a subset. Note also that when the electron has a stationary point at a particular position in reciprocal space, the time spent within an infinitesimal range Δk of this position is finite since $\dot{\gamma}\to 0$. This clearly prevents the electron from spending the same time at each position in the Brillouin zone during a finite time τ, and dynamic localization thus cannot occur. Since by Eq. (3) we have $\dot{\gamma}\propto E$, a stationary point in reciprocal space occurs when $E(t)=0$. Note that γ in Fig. 1 *does* have stationary points (e.g., at $k=x/d$ at $t=t_{10}$) and thus cannot lead to EDL.[10] The conclusion that EDL only occurs when the electric field has no zero crossings was noted earlier.[10]

In conclusion, we have considered dynamic localization assuming only the presence of a single band and the absence of decoherence. We showed that the symmetry of the periodic potential has no effect on the existence of dynamic localization or on the electric fields required to achieve it. However, the dynamics of the electrons can depend strongly on the inclusion of new terms that enter the evolution equations when the potential is asymmetric. Although these terms vanish if maximally localized Wannier functions are used, they are not negligible in general. Finally we have shown that the condition for EDL corresponds to requiring that electrons spend the same amount of time everywhere in the first Brillouin zone, irrespective of the initial condition.

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[1] D.H. Dunlap and V.M. Kenkre, Phys. Rev. B **34**, 3625 (1986).
[2] M. Holthaus, Phys. Rev. Lett. **69**, 351 (1992).
[3] J. Zak, Phys. Rev. Lett. **71**, 2623 (1993).
[4] For example, T. Meier, G. vonPlessen, P. Thomas, and S.W. Koch, Phys. Rev. Lett. **73**, 902 (1994); V.M. Axt, G. Bartels, and A. Stahl, *ibid.* **76**, 2543 (1996); J.M. Lachaine, M. Hawton, J.E. Sipe, and M.M. Dignam, Phys. Rev. B **62**, R4829 (2000).
[5] H.-F. Liu and X.-G. Zhao, Int. J. Mod. Phys. B **14**, 41 (2000).
[6] P. Domachuk, C.M. de Sterke, J. Wan, and M.M. Dignam, Phys. Rev. B **66**, 165313 (2002).
[7] M.J. Zhu, X.-G. Zhao, and Q. Niu, J. Phys.: Condens. Matter **11**, 4527 (1999).
[8] M. Holthaus and D. Hone, Phys. Rev. B **47**, 6499 (1993).
[9] X.-G. Zhao, J. Phys.: Condens. Matter **6**, 2751 (1994).
[10] M.M. Dignam and C.M. de Sterke, Phys. Rev. Lett. **88**, 046806 (2002).
[11] G. Lenz, R. Parker, M.C. Wanke, and C.M. de Sterke, Opt. Commun. **218**, 87 (2003).
[12] W. Kohn, Phys. Rev. **115**, 809 (1959).
[13] E.I. Blount, in *Solid State Physics, Advances in Research and Applications*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1961), Vol. 13.
[14] S. Kivelson, Phys. Rev. B **26**, 4269 (1982).
[15] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12 847 (1997).